Combined DAFS/crystallographic analysis for extracting the Fe local structure in a Fe/Ir(100) superlattice

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We have performed DAFS experiments at the Fe edge for studying the changes of Fe local structure in a Fe/Ir superlattice. The DAFS (diffraction anomalous fine structure) measurements were carried out at the x-ray undulator beamline BW1 (HASYLAB) and at the beamline D2AM (ESRF). For obtaining the most reliable crystallographic structure, we have refined simultaneously 3 diffraction spectra (2 at the Fe edge and 1 at the Ir edge) together with the smooth parts of 5 different DAFS data. The superlattice periodicity is 29.93Å and is made of 17 atomic planes of pure Fe plus 4 containing 30% of Ir atoms. The crystallographic structure was used for obtaining an accurate absorption correction and for separating the site-dependent XAFS-like information. To separate the XAFS-like information of Fe atoms located in the mixed Fe-Ir planes from that of those in the Fe planes, we refined simultaneously the Fourier filtered signals of the 5 normalized DAFS oscillations. Each filtered signal was weighted with the coefficients (i.e., the crystallographic phases) given by the crystallographic refinements. The results show that the DAFS spectroscopy is able to probe two planes at the interface out of the 21 of the superlattice cell. We will present the combined DAFS/crystallographic data analysis. We will also discuss the different DAFS data collection strategies and mention the experimental setups already in used at the ESRF.